

Symmetry-protected topological phases and transition in a frustrated spin- $\frac{1}{2}$ XXZ chain

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Frustrated spin-1/2 XXZ zigzag chains relevant to $\text{Rb}_2\text{Cu}_2\text{Mo}_3\text{O}_{12}$ are revisited in the light of symmetry-protected topological (SPT) phases. Using a density-matrix renormalization group method for infinite systems, we identify projective representations for four distinct time-reversal invariant SPT phases; two parity-symmetric dimer phases near the Heisenberg and XX limits and two parity-broken vector-chiral (VC) dimer phases in between. A small bond alternation in the nearest-neighbor ferromagnetic exchange coupling induces a direct SPT transition between the two distinct VC dimer phases. It is also found numerically that two Berezinskii-Kosterlitz-Thouless transitions from the gapless to the two distinct gapped VC phases meet each other at a Gaussian criticality of the same Tomonaga-Luttinger parameter value as in the $\text{SU}(2)$ -symmetric case.

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Topological orders and the quantum entanglement provide novel notions for classifying gapped quantum states beyond the conventional Landau theory [1]. These notions are indispensable for distinguishing between gapped ground states of the same symmetry group that are not adiabatically connected. The entanglement remains short-range if the gapped ground state can be described as a direct (and thus unentangled) product of wavefunctions of finite-size blocks, and is long-range otherwise [1]. Long-range entangled states may show nontrivial long-range topological orders either without any spontaneous symmetry breaking, as in Z_2 quantum spin liquids [2], or with a symmetry breaking, as in topological superconductors [3]. Short-range entangled (SRE) states can be transformed into each other without closing the energy gap. However, this transformation may necessarily break a certain symmetry. Then, this symmetry protects a topological distinction between the two SRE states. Such phases are referred to as symmetry-protected topological (SPT) phases. Well-known examples include the Haldane phase [4–7] of spin-1 chains having the time-reversal, dihedral, inversion symmetries and time-reversal invariant topological insulators [3]. The topological structure of an SPT phase with a symmetry group G is characterized by an algebra of the projective representation of G for the SRE ground state, and can thus be classified according to the group cohomology [8–11]. Some one-dimensional (1D) interacting cases including the Haldane spin chain [6, 7] and spin-1/2 ladders [12] have been demonstrated numerically.

However, a topological transition between distinct nontrivial SPT phases has not been reported yet in spin systems. This motivates us to study a simple yet more nontrivial case of a frustrated spin-1/2 chain [13, 14] including nearest-neighbor (NN) ferromagnetic ($J_1 < 0$), second-neighbor antiferromagnetic ($J_2 > 0$) exchange couplings, the relative amplitude of the NN bond al-

ternation (δ), and the XXZ-type easy-plane exchange anisotropy (Δ);

$$\begin{aligned} \hat{\mathcal{H}} = & J_1 \sum_i (1 - (-1)^i \delta) \left[\hat{S}_i^x \hat{S}_{i+1}^x + \hat{S}_i^y \hat{S}_{i+1}^y + \Delta \hat{S}_i^z \hat{S}_{i+1}^z \right] \\ & + J_2 \sum_i \left[\hat{S}_i^x \hat{S}_{i+2}^x + \hat{S}_i^y \hat{S}_{i+2}^y + \Delta \hat{S}_i^z \hat{S}_{i+2}^z \right], \end{aligned} \quad (1)$$

with a spin-1/2 operator $\hat{\mathbf{S}}_i$ at a site i . Equation (1) with $\delta = 0$ provides a minimal model for understanding the emergence of a long-range order (LRO) of the vector spin chirality, $\langle \hat{\kappa}^z \rangle = \frac{1}{N} \sum_i \langle (\hat{\mathbf{S}}_i \times \hat{\mathbf{S}}_{i+1})^z \rangle \neq 0$ with N being the number of spins [15–18], and the associated ferroelectric polarization in various quasi-1D spin-1/2 cuprate Mott insulators [17, 19–24]. A vital role of nonzero δ [25] has been proposed for a gapped vector-chiral (VC) dimer state without a quasi-LRO of a spin spiral, in accordance with experiments on $\text{Rb}_2\text{Cu}_2\text{Mo}_3\text{O}_{12}$ which has a weak crystallographic dimerization [26, 27]. This induces two pairs of time-reversal and translation invariant gapped phases with and without the inversion symmetry, each pair of which belong to the same symmetry group [25] but are expected to possess a distinct topology protected by symmetries.

In this Letter, using the infinite-size density matrix renormalization group (iDMRG) [28] method, we classify these four gapped phases of this J_1 - J_2 frustrated spin-1/2 XXZ chain model in terms of SPT phases. We also analyze the criticality of an SPT transition between two VC dimer phases, which supports the conformal field theory (CFT) [29] of the central charge $c = 1$.

The ground-state phase diagram of Eq. (1) was revealed numerically in a wide range of parameters Δ and J_1/J_2 for $\delta = 0$ [17, 18] and $\delta \neq 0$ [25] and has also been reproduced by our present iDMRG calculations. In particular, the following distinct ground states appear with decreasing Δ from unity to zero for

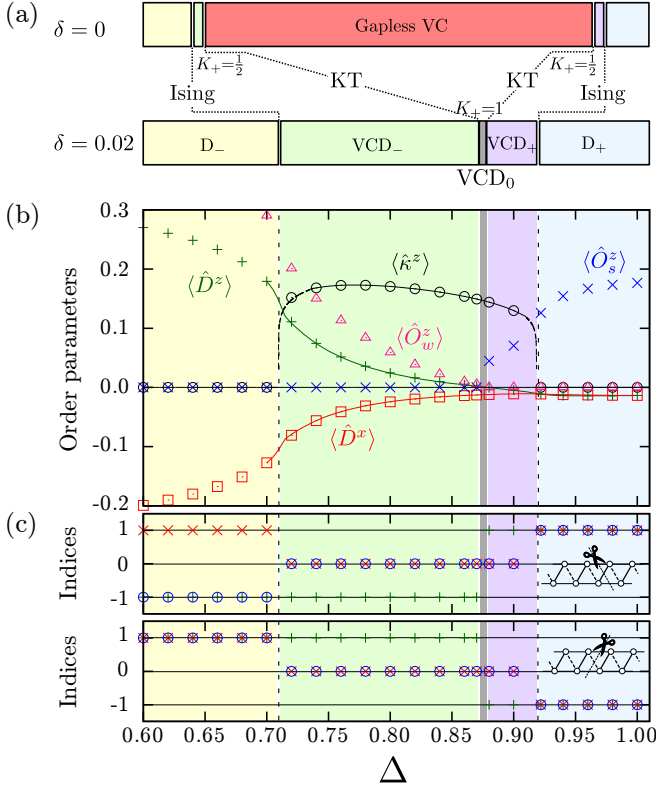


FIG. 1: (Color online) Our iDMRG results for $J_1/J_2 = -2.5$ obtained with 300 renormalized basis states ($m = 300$). (a) Phase diagrams of the Hamiltonian given by Eq. (1) for $\delta = 0$ and $\delta = 0.02$. (b) Order parameters for $\delta = 0.02$. Black, green, and red solid lines are extrapolations of the DMRG to the thermodynamic limit [25]. (c) Variations in Z_2 indices [$\beta(\Theta)$ and $\gamma(\Theta, R_{2z})$: $+$; $\beta(I)$: \times ; $\omega(R_{2x}R_{2z})$: \circ]. (Definitions are given in the text.) The upper/lower panel shows results obtained by dividing the system at a strong/weak J_1 bond.

$-2.7 \lesssim J_1/J_2 \lesssim -1.5$ [18], as shown in Fig. 1 (a) for $\delta = 0$ and $|\delta| = 0.02$, with $J_1/J_2 = -2.5$ being fixed.

i) Haldane dimer (D_+) state [18] — This is given by a Haldane state [4, 5] of the NN spin pairs that are ferromagnetically coupled with the stronger relative amplitude $1 + |\delta|$ [18, 25, 30]. In this phase, two dimer order parameters $\langle \hat{D}^x \rangle = \langle \hat{D}^y \rangle$ and $\langle \hat{D}^z \rangle$ have the same sign while the vector spin chirality vanishes, i.e., $\langle \hat{\kappa}^z \rangle = 0$, as shown in Fig. 1 (b) for $\delta = 0.02$, where $\langle \hat{D}^\alpha \rangle = \frac{1}{N} \sum_i (-1)^{i-1} \langle \hat{S}_i^\alpha \hat{S}_{i+1}^\alpha \rangle$.

ii) Vector-chiral Haldane dimer (VCD_+) state — The state preserves the relation $\langle \hat{D}^x \rangle \langle \hat{D}^z \rangle > 0$, while the parity symmetry is spontaneously broken by a LRO of the vector spin chirality; $\langle \hat{\kappa}^z \rangle \neq 0$.

iii) Vector-chiral dimer (VCD_-) state — This is similar to the VCD_+ state, except the sign of $\langle \hat{D}^z \rangle$ is reversed and thus $\langle \hat{D}^x \rangle \langle \hat{D}^z \rangle < 0$.

iv) Gapless vector-chiral states — The z -component dimer order parameter vanishes, $\langle \hat{D}^z \rangle = 0$, while the

LRO of vector spin chirality survive, i.e. $\langle \hat{\kappa}^z \rangle \neq 0$. The other components $\langle \hat{D}^x \rangle = \langle \hat{D}^y \rangle$ are zero for $\delta = 0$ (gapless VC phase) [15–17], but are finite for $\delta \neq 0$ (critical VCD_0 state) [25]. For $\delta \neq 0$, the condition of $\langle \hat{D}^z \rangle = 0$ for the VCD_0 state is satisfied only at a single direct transition point between VCD_\pm phases, although a possibility that it extends to a narrow gray hatched region in Fig. 1(b) has not been ruled out.

v) Even-parity dimer (D_-) state — This has $\langle \hat{D}^x \rangle \langle \hat{D}^z \rangle < 0$, while the vector spin chirality eventually vanishes, i.e., $\langle \hat{\kappa}^z \rangle = 0$.

The D_\pm phases belong to the same symmetry group G as that of the Hamiltonian, $G_{\mathcal{H}}$, which contains $U(1)$ for the spin symmetry, the group T of translations by integer multiples of two sites, the dihedral point group $D_{2h} = D_2 \times C_1$ with $C_1 = \{E, I\}$ and the spatial inversion I about a bond center, and the anti-unitary group $\{E, \Theta\}$ with the identity E and the time-reversal Θ . The VCD_\pm and VCD_0 also have a common symmetry group G_{VCD} , which can be derived by replacing D_{2h} with C_{2v} where the inversion symmetry is lost while two mirror planes are preserved. Clearly, the $D_+ - VCD_+$ and $D_- - VCD_-$ transitions are symmetry-breaking transitions, which belong to the Ising criticality described with the $c = 1/2$ CFT [25]. In particular, it breaks the I symmetry while preserving the mirror symmetry including the z axis, e.g., IR_{2x} with the π rotation R_{2i} about the i axis. In contrast, the $VCD_+ - VCD_-$ transition is not if it occurs as a direct transition. We probe this $VCD_+ - VCD_-$ transition only from the sign change of $\langle \hat{D}^x \rangle \langle \hat{D}^z \rangle$ but also from two string order parameters [31, 32] O_n^z ($n = 1, 2$) defined by

$$O_n^z = - \lim_{r \rightarrow \infty} \langle (\hat{S}_n^z + \hat{S}_{n+1}^z) e^{i\pi \sum_{k=n+2}^{2r+n-1} \hat{S}_k^z} (\hat{S}_{2r+n}^z + \hat{S}_{2r+n+1}^z) \rangle. \quad (2)$$

Only $\langle O_s^z \rangle$ ($\langle O_w^z \rangle$) with a pair of sites n and $n+1$ belonging to different dimer units (see Table I) and thus forming a strong (weak) bond becomes long-range in the $D_{+(-)}$ and $VCD_{+(-)}$ phases, as shown in Fig. 1(b) and in the previous work [25].

This change in the string order parameters is consistent with a change in the degeneracy of the lowest entanglement spectrum. In two rightmost columns of Table I, we show the degeneracy n_s (n_w) of the lowest bipartite entanglement spectrum, or in other words, that of the entanglement Hamiltonian [33] $\hat{\mathcal{H}}_s$ ($\hat{\mathcal{H}}_w$) obtained through iDMRG calculations under the condition that the whole spin chain is divided at a strong (weak) bond: $n_s = 1$ and $n_w = 2$ for the D_+ and VCD_+ phases, while $n_s = 2$ and $n_w = 1$ for the D_- and VCD_- phases. This topological change occurring only at the $VCD_+ - VCD_-$ transition indicates that the D_\pm phases are not adiabatically connected and neither are the VCD_\pm phases, as long as the symmetry of these phases is respected.

Nature of these gapped phases can be captured by classifying them as SPT phases, according to the 1D repre-

TABLE I: (Color online) Ten Z_2 indices for the projective representation of $G_{\mathcal{H}}$ in D_{\pm} , VCD_{\pm} , and $VCND$ [25] ground states, the degeneracy n_s/n_w of the lowest entanglement spectrum $\zeta_0 = -\log w_0$ and the schematic picture of the ground state of $\hat{\mathcal{H}}_s/\hat{\mathcal{H}}_w$ when dividing the system at a stronger/weaker (left/right panel) bond. The emergence of -1 in β , γ and/or ω points to a double topological degeneracy in the lowest entanglement spectrum. Orange, green and pink pairs indicate antisymmetric $[(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)/\sqrt{2}]$, symmetric $[(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle)/\sqrt{2}]$ and mixed $[(e^{i\theta/2}|\uparrow\downarrow\rangle + e^{-i\theta/2}|\downarrow\uparrow\rangle)/\sqrt{2}]$ units of dimers which show $\langle \hat{D}_j^z \rangle \langle \hat{D}_j^x \rangle > 0$ and $\langle \hat{D}_j^z \rangle \langle \hat{D}_j^x \rangle < 0$, respectively. These parity symmetries are broken in pink pairs due to presence of vector-chiral order. The twofold Kramers degeneracy arising from the edge is denoted by a pair of black up and down arrows.

Phase	p	$\alpha(p)$	$\alpha(h)$		$\beta(p)$	$\beta(\Theta)$	$\gamma(p, h)$		$\gamma(\Theta, h)$		$\omega(R_{2x}, R_{2z})$	Degeneracy n_s/n_w of the ground state of $\hat{\mathcal{H}}_s/\hat{\mathcal{H}}_w$			
			R_{2x}	R_{2z}			R_{2x}	R_{2z}	R_{2x}	R_{2z}		n_s		n_w	
D_+	I	-1	$+1$	$+1$	± 1	± 1	± 1	± 1	± 1	± 1	± 1	1		2	
D_-	I	$+1$	-1	$+1$	$+1$	∓ 1	$+1$	∓ 1	∓ 1	∓ 1	∓ 1	2		1	
VCD_+	IR_{2x}	-1	0	$+1$	$+1$	± 1	0	$+1$	0	± 1	0	1		2	
VCD_-	IR_{2x}	-1	0	$+1$	$+1$	∓ 1	0	$+1$	0	∓ 1	0	2		1	
$VCND$	IR_{2x}	-1	0	$+1$	$+1$	0	0	$+1$	0	0	0	1		1	

representations and the factor systems for the projective representation of the symmetry group G of each ground state. Let us consider the set of Z_2 indices, α 's, β 's, γ 's, and ω 's listed in Table I [6, 7, 9] for the symmetry group $G_{\mathcal{H}}$ of the Hamiltonian, so that the symmetry group G of all the ground states of our interest can be given by a subgroup of $G_{\mathcal{H}}$. These indices are determined from

$$\sum_{jj'} (T_I(h_p))_{ii', jj'} (D_p)_{j, j'} = \alpha(p) (D_p)_{i, i'}, \quad (3)$$

$$\sum_{jj'} (T_{\Theta}(h_{\Theta}))_{ii', jj'} (D_{\Theta})_{j, j'} = \alpha(\Theta) (D_{\Theta})_{i, i'}, \quad (4)$$

$$\sum_{jj'} (T(h))_{ii', jj'} (\mathcal{U}_h)_{j, j'} = \alpha(h) (\mathcal{U}_h)_{i, i'}, \quad (5)$$

$$\beta(p) = \text{Tr}[D_p (D_p^{-1})^t]/m, \quad \beta(\Theta) = \text{Tr}[D_{\Theta} D_{\Theta}^*]/m, \quad (6)$$

$$\gamma(p, h) = \text{Tr}[\mathcal{U}_h D_p \mathcal{U}_h^{\dagger} D_p^{-1}]/m, \quad (7)$$

$$\gamma(\Theta, h) = \text{Tr}[\mathcal{U}_h D_{\Theta} (\mathcal{U}_h^*)^{-1} D_{\Theta}^{-1}]/m, \quad (8)$$

$$\omega(h', h) = \text{Tr}[\mathcal{U}_h \mathcal{U}_{h'} \mathcal{U}_h^{-1} \mathcal{U}_{h'}^{-1}]/m, \quad (9)$$

where h is taken from a minimal set of generators of the local unitary subgroup H_{LU} of the whole symmetry group G , $p = Ih_p$ is a direct product of the inversion I and $h_p = E$ or $R_{2x} \in H_{LU}$, $\Theta = h_{\Theta}K$ is a direct product of the complex conjugate operator K and $h_{\Theta} = R_{2y} \in H_{LU}$. We have also introduced transfer matrices for a unit cell including two spins

$$(T_I(h))_{ii', jj'} = \sum_{s_1 s_2 s'_1 s'_2} (A^{*(s_1 s_2)})_{ij} (U_h)_{s_1 s_2 s'_1 s'_2} (A^{(s'_1 s'_2)})_{i' j'}, \quad (10)$$

$$(T_{\Theta}(h))_{ii', jj'} = \sum_{s_1 s_2 s'_1 s'_2} (A^{*(s_1 s_2)})_{ij} (U_h)_{s_1 s_2 s'_1 s'_2} (A^{*(s'_1 s'_2)})_{i' j'}, \quad (11)$$

$$(T(h))_{ii', jj'} = \sum_{s_1 s_2 s'_1 s'_2} (A^{*(s_1 s_2)})_{ij} (U_h)_{s_1 s_2 s'_1 s'_2} (A^{(s'_1 s'_2)})_{i' j'}, \quad (12)$$

where the $m \times m$ matrix $A^{(s_1 s_2)}$ represents in the Schmidt bases the state within the translation unit having the two-spin degrees of freedom, $(s_1 s_2)$, in the translationally invariant matrix product state (MPS) [34–36] $|\Psi\rangle_i = \sum_{s_1 s_2 j} (A^{(s_1 s_2)})_{ij} |s_1 s_2\rangle \otimes |\Psi\rangle_j$ of the entanglement Hamiltonian satisfying the orthonormal condition ${}_i \langle \Psi | \Psi \rangle_j = \delta_{ij}$ [37]. Right eigenvectors of transfer matrices in Eqs. (3), (4), and (5) are the representation matrices of I , Θ , and h , respectively, in the Schmidt bases. (See Supplementary materials.) The arbitrary phases of $\mathcal{U}_{R_{2x}}$ and $\mathcal{U}_{R_{2z}}$ are fixed by $\mathcal{U}_{R_{2x}}^2 = \mathcal{U}_{R_{2z}}^2 = \mathbb{1}$. Note that for Θ -invariant states, i.e., $|\alpha(\Theta)| = 1$, $\alpha(\Theta)$ just takes arbitrary $U(1)$ phase depending on that of $A^{(s_1 s_2)}$ and thus is not important. The results are summarized in Table I. Because of the unbroken $U(1)_z$ symmetry, the 1D representation $\alpha(R_{2z}) = 1$ leading to R_{2z} -even states is rather obvious in all the phases shown in Table I, and thus is not particularly mentioned below.

From two 1D representations $\alpha(I)$ and $\alpha(R_{2x})$, the D_+ ground state of the whole spin chain is I -odd and R_{2x} -even. All the other Z_2 indices take the same value; $\beta(I) = \beta(\Theta) = \gamma(I, h) = \gamma(\Theta, h) = \omega(R_{2x}, R_{2z}) = +(-)1$ with $h = R_{2x}, R_{2z}$ if the spin chain is cut at a strong (weak) bond. This is consistent with the nondegeneracy $n_s = 1$ and the twofold degeneracy $n_w = 2$ in the entanglement spectrum, and indicates that this SPT phase is protected by I , Θ , and D_2 symmetries [6, 7]. This phase has the same Z_2 indices as the Affleck-Kennedy-Lieb-Tasaki (AKLT) state [5, 38].

The D_- phase is I -even ($\alpha(I) = +1$) and R_{2x} -odd ($\alpha(R_{2x}) = -1$). Whichever bond the spin chain is cut at, $\beta(I) = \gamma(I, R_{2x}) = +1$, indicating that the I symmetry no longer protects the topological degeneracy. All the other indices take the same value; $\beta(\Theta) = \gamma(I, R_{2z}) =$

$\gamma(\Theta, h) = \omega(R_{2x}, R_{2z}) = -(+)1$ if the spin chain is cut at a strong (weak) bond. This is consistent with $n_s = 2$ and $n_w = 1$, and indicates that this SPT phase is protected by Θ and D_2 symmetries. This phase has the same Z_2 indices as a direct product of the even-parity dimer state, $(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle)/\sqrt{2}$ [39].

Let us proceed to the VCD_{\pm} phases. These states respect the IR_{2x} symmetry and are IR_{2x} -odd, while they break the I and R_{2x} symmetries, as seen from $\alpha(IR_{2x}) = -1$ and $\alpha(R_{2x}) = 0$. (Note that the D_{\pm} states are also IR_{2x} -odd as $\alpha(IR_{2x}) = \alpha(I)\alpha(R_{2x}) = -1$.) The VCD_{\pm} states have the same topological degeneracy in the entanglement spectrum as D_{\pm} , respectively, but they are no longer protected by the I and D_2 symmetry, and not even by the IR_{2x} symmetry since $\beta(IR_{2x}) = \gamma(IR_{2x}, R_{2z}) = +1$ always holds. The sign of $\beta(\Theta) = \gamma(\Theta, R_{2z})$ depends on the way of dividing the spin chain and are opposite between the VCD_+ and VCD_- phases, and the minus sign appears when the entanglement spectrum is twofold degenerate. Hence, VCD_{\pm} phases are classified into distinct SPT phases, whose distinction is protected by the Θ symmetry. Indeed, once, the Neel LRO is realized in addition to the VCD orders, the Θ symmetry is broken [25] and the topological degeneracy is lost completely (Table I).

Finally, we clarify the nature of this $VCD_+ - VCD_-$ SPT phase transition. Figure 2 (a) shows the dependence of the correlation length $\xi = -1/\log(|w_1/w_0|)$ on the dimension m of the Schmidt bases in the vicinity of $VCD_+ - VCD_-$ transition, where w_n is the $(n+1)$ -th-largest (in terms of absolute value) eigenvalue of the transfer matrix $T(E)$. This indicates the strongest enhancement of ξ at $\Delta = 0.88$, indicating a proximity to the criticality in reasonable agreement with the sign change of $\langle \hat{D}^z \rangle$ at $\Delta = 0.879(1)$. The scaling behavior of the entanglement entropy versus ξ in the form of $S = \frac{c}{6} \log \xi + \text{const.}$ shown in Fig. 2 (b) is consistent, within the numerical accuracy, with the $c = 1$ CFT [29]. We also estimate the Tomonaga-Luttinger (TL) parameter K_+ for the gapless VCD_0 state [18, 25] to be unity (1.00(1)), the same value as for the TL liquid in the $SU(2)$ NN antiferromagnetic spin- $\frac{1}{2}$ chain, by fitting a spatial decay of the transverse equal-time spin correlation with the leading term as $\langle \hat{S}_0^x \hat{S}_\ell^x \rangle \simeq A e^{iQ\ell} |\ell|^{-1/(2K_+)}$, as shown in Fig. 2 (c) and (d). If we applying the heuristic bosonization analysis [15] to our model [25], this value $K_+ = 1$ is indeed required for having a direct continuous transition between the VCD_{\pm} phases [25]. This supports the scenario that two Berezinskii-Kosterlitz-Thouless (BKT) transitions at $K_+ = \frac{1}{2}$ from the gapless VC to gapped VCD_{\pm} phases in the case of $\delta = 0$ shift and meet each other at the $K_+ = 1$ line in the case of $\delta \neq 0$ (see Fig.1 (a)): the change of the critical K_+ value is caused by an appearance of the more relevant perturbation of the bond alternation [25]. This contrasts to the case of the transition between the large- D and

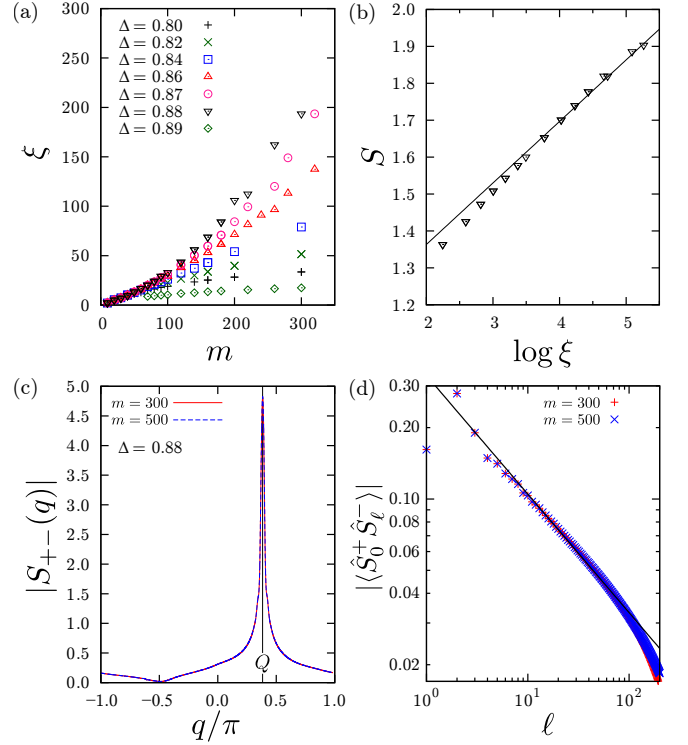


FIG. 2: (Color online) (a) Correlation length ξ as a function of m in the vicinity of the $VCD_+ - VCD_-$ phase boundary. (b) Scaling of the entanglement entropy S as a function of correlation length ξ at $\Delta = 0.88$. The solid line represents the $c = 1$ line. (c) The Fourier transform $S_{+-}(q)$ of $\langle \hat{S}_0^+ \hat{S}_\ell^- \rangle$ ($1 \leq \ell \leq 128$). It exhibits a peak at $q = Q$ with $Q/\pi = 0.383$ denoted by the solid line. (d) Logarithmic plot of $|\langle \hat{S}_0^+ \hat{S}_\ell^- \rangle|$. The solid curve shows the scaling function given in the text with $A = 0.332(4)$ and $K_+ = 1.00(1)$, where the number in a parenthesis means the standard error coming from the least-square fitting in the range $5 \leq \ell \leq 100$. The downward deviation for $\ell > \xi \sim 100 - 200$ is due to the effect of the truncation.

Haldane phases, which has a simple Gaussian criticality with a weak universality [41, 42]. Analytically describing the possible coincidence of two BKT transitions at the $K_+ = 1$ Gaussian criticality is left open.

Since the model parameters are at least close to those for the spin-gapped spin-1/2 chain compound $Rb_2Cu_2Mo_4O_{12}$ [25–27], it would be intriguing to experimentally find these SPT phases and the SPT transition by probing a gap closing under physical and/or chemical pressure.

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- [1] X. Chen, Z.-C. Gu, and X.-G. Wen, Phys. Rev. B **82**, 155138 (2010).
- [2] X.-G. Wen, Phys. Rev. B **65**, 165113 (2002).
- [3] M. Z. Hasan and C. L. Kane, Rev. Mod. Phys. **82**, 3045 (2010).
- [4] F.D.M. Haldane, Phys. Lett. 93A, 464 (1983); Phys. Rev. Lett. **50**, 1153 (1983).
- [5] I. Affleck, T. Kennedy, E. H. Lieb, and H. Tasaki, Phys. Rev. Lett. **59**, 799 (1987).
- [6] F. Pollmann, A.M. Turner, E. Berg, and M. Oshikawa, Phys. Rev. B **81**, 064439 (2010).
- [7] F. Pollmann and A.M. Turner, Phys. Rev. B **86**, 125441 (2012).
- [8] Z.-X. Liu, X. Chen, and X.-G. Wen, Phys. Rev. B **84**, 195145 (2011).
- [9] X. Chen, Z.-C. Gu, and X.-G. Wen, Phys. Rev. B **84**, 235128 (2011).
- [10] X. Chen, Z.-C. Gu, Z.-X. Liu, and X.-G. Wen, Science **338**, 1604 (2012); Phys. Rev. B **87**, 155114 (2013).
- [11] N. Schuch, D. Pérez-García, and I. Cirac, Phys. Rev. B **84**, 165139 (2011).
- [12] Z.-X. Liu, Z.-B. Yang, Y.-J. Han, W. Yi, and X.-G. Wen, Phys. Rev. B **86**, 195122 (2012).
- [13] A.V. Chubukov, Phys. Rev. B **44**, 4693 (1991).
- [14] P. Lecheminant, in *Frustrated spin systems*, edited by H. T. Diep (World-Scientific, Singapore, 2005), Review chapter; arXiv:cond-mat/0306520.
- [15] A.A. Nersisyan, A.O. Gogolin, and F.H.L. Eßler, Phys. Rev. Lett. **81**, 910 (1998).
- [16] T. Hikihara, M. Kaburagi, and H. Kawamura, Phys. Rev. B **63**, 174430 (2001).
- [17] S. Furukawa, M. Sato, and S. Onoda, Phys. Rev. Lett. **105**, 257205 (2010).
- [18] S. Furukawa, M. Sato, S. Onoda, and A. Furusaki, Phys. Rev. B **86**, 094417 (2012).
- [19] T. Masuda, A. Zheludev, B. Roessli, A. Bush, M. Markina, and A. Vasiliev, Phys. Rev. B **72**, 014405 (2005).
- [20] S. Park, Y. J. Choi, C. L. Zhang, and S-W. Cheong, Phys. Rev. Lett. **98**, 057601 (2007).
- [21] M. Enderle *et al.*, Europhys. Lett. **70**, 237 (2005).
- [22] Y. Naito, K. Sato, Y. Yasui, Y. Kobayashi, Y. Kobayashi, and M. Sato, J. Phys. Soc. Jpn. **76**, 023708 (2007).
- [23] Y. Yasui, M. Sato, and I. Terasaki, J. Phys. Soc. Jpn. **80**, 033707 (2011).
- [24] A. U. B. Wolter, F. Lipps, M. Schäpers, S.-L. Drechsler, S. Nishimoto, R. Vogel, V. Kataev, B. Büchner, H. Rosner, M. Schmitt, M. Uhlarz, Y. Skourski, J. Wosnitza, S. Süllo, and K. C. Rule, Phys. Rev. B **85**, 014407 (2012).
- [25] H. Ueda and S. Onoda, Phys. Rev. B **89**, 024407 (2014).
- [26] M. Hase, H. Kuroe, K. Ozawa, O. Suzuki, H. Kitazawa, G. Kido, and T. Sekine, Phys. Rev. B **70**, 104426 (2004).
- [27] Y. Yasui, Y. Yanagisawa, R. Okazaki, I. Terasaki, Y. Yamaguchi, and T. Kimura, J. Appl. Phys. **113**, 17D910 (2013).
- [28] I. P. McCulloch, arXiv:0804.2509
- [29] P. Di Francesco, P. Mathieu, and D. Sénéchal, *Conformal Field Theory* (Springer, New York, 1996).
- [30] C. Itoi and S. Qin, Phys. Rev. B **63**, 224423 (2001).
- [31] M. den Nijs and K. Rommelse, Phys. Rev. B **40**, 4709 (1989).
- [32] H. Tasaki, Phys. Rev. Lett. **66**, 798 (1991).
- [33] Hui Li and F. D. M. Haldane, Phys. Rev. Lett. **101**, 010504 (2008).
- [34] S. Östlund and S. Rommer, Phys. Rev. Lett. **75**, 3537 (1995).
- [35] S. Rommer and S. Östlund, Phys. Rev. B **55**, 2164 (1997).
- [36] U. Schollwöck, Ann. Phys. (NY) **326**, 96 (2011).
- [37] Actually, we first adopted an infinite MPS $|\Psi\rangle$ invariant under the four-site translation in our iDMRG calculation. Then, we checked the state is invariant under two-site translations, namely, $|\Psi\rangle = \hat{T}|\Psi\rangle$.
- [38] The AKLT state on the $S = 1/2$ chain is described by a product state of the following translation-unit matrix $A_w^{(s_1 s_2)}$ or $A_s^{(s_1 s_2)}$ in the Schmidt bases obtained by dividing the whole system at a weak or strong J_1 bond; $A_w^{(\uparrow\uparrow)} = \sqrt{\frac{2}{3}}\sigma^+$, $A_w^{(\downarrow\downarrow)} = -\sqrt{\frac{2}{3}}\sigma^-$ and $A_w^{(\uparrow\downarrow)} = A_w^{(\downarrow\uparrow)} = -\sqrt{\frac{1}{6}}\sigma^z$. $A_s^{(s_1 s_2)}$ is readily obtained by applying the singular value decomposition to $A_w^{(s_1 s_2)}$; using singular vectors and values in $(A_w^{(s_1 s_2)})_{\alpha_1 \alpha_2} = \sum_{\beta=1}^4 X_{\alpha_1 s_1, \beta} W_{\beta, \beta} Y_{\beta, s_2 \alpha_2}^\dagger$, we can take $(A_s^{(s_1 s_2)})_{\beta_1 \beta_2} = \sum_{\alpha} W_{\beta_1, \beta_1} Y_{\beta_1, s_1 \alpha}^\dagger X_{\alpha s_2, \beta_2}$.
- [39] $A_w^{(s_1 s_2)}$ of the direct product state of $(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle)/\sqrt{2}$ can be written as $A_w^{(\uparrow\uparrow)} = A_w^{(\downarrow\downarrow)} = \begin{pmatrix} 0 \end{pmatrix}$, $A_w^{(\uparrow\downarrow)} = A_w^{(\downarrow\uparrow)} = \begin{pmatrix} \frac{1}{\sqrt{2}} \end{pmatrix}$. $A_s^{(s_1 s_2)}$ of this state can be obtained in the same way as explained in [38]. These $A_{w/s}^{(s_1 s_2)}$ lead to the same Z_2 indices as in the D_- state. $A_{w/s}^{(s_1 s_2)}$ of the direct product state of $(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)/\sqrt{2}$, namely, the Majumdar-Ghosh state [40], can be obtained by rotating every other spins about the z -axis by π . This resulting Z_2 indices are the same as in the D_+ state, except with the interchange of “w” and “s”.
- [40] C. K. Majumdar and D. K. Ghosh, J. Math. Phys. **10**, 1399 (1969).
- [41] M. Yamanaka, Y. Hatsugai, and M. Kohmoto, Phys. Rev. B **48**, 9555 (1993).
- [42] K. Hida, J. Phys. Soc. Jpn. **62**, 1466 (1993).

**SUPPLEMENTARY MATERIALS FOR “SYMMETRY-PROTECTED TOPOLOGICAL PHASES AND
TRANSITION IN A FRUSTRATED SPIN- $\frac{1}{2}$ XXZ CHAIN”**

We provide details of a correspondence between the right eigenvector of the transfer matrix given by Eq. (5) in the main text and the representation matrix in the Schmidt bases. Schmidt bases of a finitely correlated ground state for a uniform one-dimensional system in the thermodynamic limit can be represented by an infinite matrix product state with sufficiently large dimension m :

$$|\Psi\rangle_i = \sum_{\{s_k\}} \left[\left(\prod_{k=1}^{+\infty} A^{(s_k)} \right) v \right]_i |\{s_k\}\rangle, \quad (1)$$

where $A^{(s)}$ and v are an m -dimensional matrix and vector. The gauge of $A^{(s)}$ can be chosen to be $\sum_s A^{(s)} A^{\dagger(s)} = \mathbb{1}$. The vector v is determined to suit the orthonormal condition, ${}_i\langle\Psi|\Psi\rangle_j = \delta_{ij}$. The bases have a translation symmetry given by $|\Psi\rangle_i = \sum_s (A^{(s)})_{ij} |s\rangle \otimes |\Psi\rangle_j$.

Let's consider a representation matrix of a local unitary operation, $\hat{U} = \prod_{k=1}^{+\infty} \sum_{s_k s'_k} (U_h)_{s_k s'_k} |s_k\rangle\langle s'_k|$, in the Schmidt bases, namely $(\mathcal{U}_h)_{ii'} = {}_i\langle\Psi|\hat{U}|\Psi\rangle_{i'}$:

$$\begin{aligned} {}_i\langle\Psi|\hat{U}|\Psi\rangle_{i'} &= \sum_{jj'} \left[\prod_{k=1}^{+\infty} \left(\sum_{s_k s'_k} (U_h)_{s_k s'_k} A^{*(s_k)} \otimes A^{(s'_k)} \right) \right]_{ii', jj'} (v^*)_j (v)_{j'}, \\ &= \sum_{jj'} \left[\prod_{k=1}^{+\infty} T(h) \right]_{ii', jj'} (v^*)_j (v)_{j'}, \end{aligned} \quad (2)$$

where the definition of the transfer matrix $T(h)$ is given by Eq. (12) in the main text. If the ground state is invariant under the unitary operation and is not a cat state, the norm of dominant eigenvalue $\alpha(h)$ of the transfer matrix $T(h)$ becomes unity and unique. In this case, $\prod_{k=1}^{+\infty} T(h)$ can be decomposed as $u_h (\prod_{k=1}^{+\infty} \alpha(h)) v_h^\dagger$, where u_h (v_h) is the right (left) eigenvector of $T(h)$ corresponding to $\alpha(h)$. Using this relation, we obtain

$${}_i\langle\Psi|\hat{U}|\Psi\rangle_{i'} = (u_h)_{ii'} \left(\prod_{k=1}^{+\infty} \alpha(h) \right) \left[\sum_{jj'} (v_h^*)_{jj'} (v^*)_j (v)_{j'} \right] = (u_h)_{ii'} \times \text{const.}, \quad (3)$$

where the constant is $(\prod_{k=1}^{+\infty} \alpha(h)) \left[\sum_{jj'} (v_h^*)_{jj'} (v^*)_j (v)_{j'} \right]$. This constant can be removed by redefining of u_h and v_h , because there is an arbitrary property in the biorthogonal condition of $v_h^\dagger u_h = 1$. Thus, we can obtain the representation matrix by reshaping the right eigenvector, as $(\mathcal{U}_h)_{i,i'} = (u_h)_{ii'}$.